Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION3.str

chain nodes : 9 10 23 24 25 26 27 28 29 30 31 34 35 36 ring nodes : 1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 chain bonds : 2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 22-26 31-34 34-35 ring bonds : 1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22 exact/norm bonds : 1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 20-31 exact bonds : 4-17 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34 34 - 35normalized bonds : 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
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L10 STRUCTURE UPLOADED

=> s 110 full

FULL SEARCH INITIATED 11:02:52 FILE 'REGISTRY'

2 SEA SSS FUL L10

FULL SCREEN SEARCH COMPLETED -66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS

SEARCH TIME: 00.00.01

=> file caplus

L11

COST IN U.S. DOLLARS

SINCE FILE TOTAL

> ENTRY 172.10

SESSION 864.35

2 ANSWERS

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:02:55 ON 16 JUL 2007

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FILE COVERS 1907 - 16 Jul 2007 VOL 147 ISS 4 FILE LAST UPDATED: 15 Jul 2007 (20070715/ED)

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=> s 111

L12 1 L11 ·

=> d ibib hitstr 1

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:395400 CAPLUS <<LOGINID::20070716>>

DOCUMENT NUMBER: 142:412928

TITLE: Heat-stable diketopyrrolopyrrole pigment mixtures for

cosmetics

INVENTOR(S): Wallquist, Olof; Lenz, Roman; Feiler, Leonhard;

Dueggeli, Mathias; Yousaf, Taher; De Keyzer, Gerardus

PATENT ASSIGNEE(S): . Ciba Specialty Chemicals Holding Inc., Switz. SOURCE:

PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
     WO 2005040284
                                 20050506
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                                             WO 2004-EP52426
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     US 2007028807
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PRIORITY APPLN. INFO.:
                                              CH 2003-1817
                                                                  Α
                                                                     20031023
                                              WO 2004-EP52426
                                                                     20041004
OTHER SOURCE(S):
                          MARPAT 142:412928
IT
     850566-77-7P
     RL: COS (Cosmetic use); IMF (Industrial manufacture); MOA (Modifier or
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     (Biological study); PREP (Preparation); USES (Uses)
        (dark red pigment; production of heat-stable diketopyrrolopyrrole pigment
        mixts. for cosmetics)
RN
     850566-77-7 CAPLUS
CN
     Pyrrolo[3,4-c]pyrrole-1,4-dione, 3-(4-chlorophenyl)-2,5-dihydro-6-[4-
     (octadecylthio)phenyl] - (9CI) (CA INDEX NAME)
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CN Pyrrolo[3,4-c]pyrrole-1,4-dione, 3-(4-chlorophenyl)-6-[4-(decylthio)phenyl]-2,5-dihydro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil reg COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY SESSION

4.09 868.44

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20

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 JUL 2007 HIGHEST RN 942400-66-0 DICTIONARY FILE UPDATES: 15 JUL 2007 HIGHEST RN 942400-66-0

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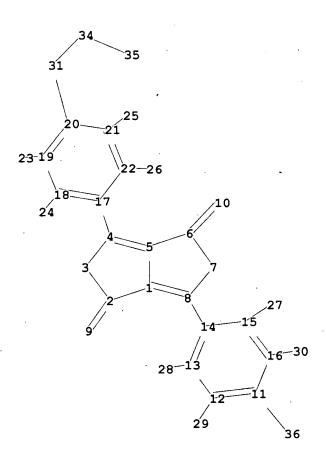
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> $\label{thm:local_correction} \begin{tabular}{ll} $$ $C:\Program $Files\strut^2 = 10576703\correction 4.strut^2 = 10576703\corr$



chain nodes : 9 10 23 24 25 26 27 28 29 30 31 34 35 36 ring nodes : 1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 chain bonds : 2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 22-26 31-34 34-35 ring bonds : 1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22 exact/norm bonds : 1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 20-31 exact bonds : 4-17 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34 normalized bonds : 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 36:CLASS 36:CLASS 36:CLASS

L13 STRUCTURE UPLOADED

=> s 113 full FULL SEARCH INITIATED 11:03:33 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -66 TO ITERATE

100.0% PROCESSED

66 ITERATIONS

2 ANSWERS

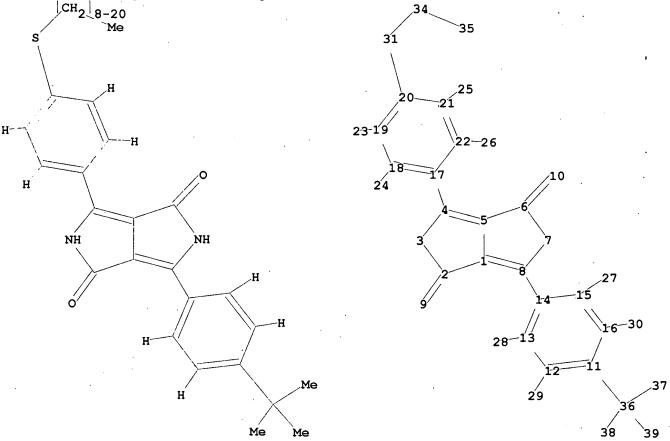
SEARCH TIME: 00.00.01

L14

2 SEA SSS FUL L13

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION6.str



chain nodes :

9 10 23 24 25 26 27 28 29 30 31 34 35 36

ring nodes :

1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20

chain bonds :

2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25

22-26 31-34 34-35 36-37 36-38 36-39

ring bonds :

1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 20-31

4-17 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34

10/576,703 REACTION SEARCH.

34-35 36-37 36-38 36-39

normalized bonds :

11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21. 21-22

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom

22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS

31:CLASS

34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS

L15 STRUCTURE UPLOADED

=> s 115 full

FULL SEARCH INITIATED 11:03:52 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 151 TO ITERATE

100.0% PROCESSED 151 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L16 1 SEA SSS FUL L15

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION7.str

chain nodes : 9 10 23 24 25 26 27 28 29 30 31 34 35 36 43 44 45 ring nodes : 1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 21 22 40 41 42 chain bonds : 2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25 22-26 31-34 34-35 36-37 38-43 39-44 40-45 41-46 42-47 ring bonds : 1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22 37-38 37-42 38-39 39-40 40-41 41-42 exact/norm bonds : 1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 11-36 20-31 exact bonds : 4-17 8-14 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34 34-35 38-43 39-44 40-45 41-46 42-47 normalized bonds : 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22 37-38 37-42 38-39 39-40 40-41 41-42

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom

22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS

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45:CLASS 46:CLASS 47:CLASS

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION7.str

chain nodes : 9 10 23 24 25 26 27 28 29 30 31 34 35 36 43 44 45 46 47 ring nodes : 1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 21 22 37 38 39 40 41 42 chain bonds : 2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25 22-26 31-34 34-35 36-37 38-43 39-44 40-45 41-46 42-47 ring bonds : 1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22 37-38 37-42 38-39 39-40 40-41 41-42 exact/norm bonds : 1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 11-36 20-31 36-37 exact bonds : 4-17 8-14 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34 34-35 38-43 39-44 40-45 41-46 42-47 normalized bonds :

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 35:CLASS 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS 47:CLASS 47:CLASS

L17 STRUCTURE UPLOADED

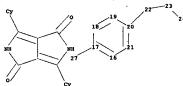
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100.0% PROCESSED 67 ITERATIONS 1 ANSWERS SEARCH TIME: 00.00.01

L18 · 1 SEA SSS FUL L17

10/576,703 REACTION SEARCH

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\RXN222222222222222.str



chain nodes :

9 10 11 12 22 23 24 27

ring nodes :

1 2 3 4 5 6 7 8 16 17 18 19 20 21

chain bonds :

2-9 4-11 6-10 8-12 17-27 20-22 22-23 23-24

ring bonds :

1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 20-22

exact bonds :

17-27 22-23 23-24

normalized bonds :

16-17 16-21 17-18 18-19 19-20 20-21

G1:H, CH3, CF3, CN, X

G2:C,S,N

G3:Cb,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom 20:CLASS 21:Atom 22:CLASS

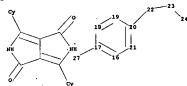
23:CLASS 24:CLASS

27:CLASS

L1 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\RXN22.str





10/576,703 REACTION SEARCH

```
chain nodes :
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ring nodes :
1 2 3 4 5 6 7 8 16 17 18 19 20
chain bonds :
2-9 4-11 6-10 8-12 17-27 20-22 22-23 23-24
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 20-22
exact bonds :
17-27 22-23 23-24
normalized bonds :
16-17 16-21 17-18 18-19 19-20 20-21
G1:H, CH3, CF3, CN, X.
G2:C,S,N
G3:Cb,Ak
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom 20:CLASS 21:Atom 22:CLASS
23:CLASS 24:CLASS
27:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 16
L2 STRUCTURE UPLOADED
=> s 12 full
FULL SEARCH INITIATED 13:56:35 FILE 'CASREACT'
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM
                                                        0 DOCUMENTS
100.0% DONE 0 VERIFIED 0 HIT RXNS
                                                                   0 DOCS
SEARCH TIME: 00.00.01
L3
             O SEA SSS FUL L2 ( O REACTIONS)
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\RXN111111.str
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July 17, 2007

```
chain nodes :
9 10 11 12 13 14 15 16 19 21 23
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
2-9 4-11 6-10 8-12 13-14
                          13-19 13-21 15-16 21-23
ring bonds :
1-2 1-5 1-8 2-3 3-4
                      4-5
                           5-6
                               6-7 7-8
exact/norm bonds :
                               4-11 5-6 6-7 6-10 7-8
1-2 1-5 1-8 2-3 2-9
                           4-5
                      3-4
                                                       8-12
13-21 15-16 21-23
```

G1:H,CH3,CF3,CN,X,[*1]

G2:C,S,N

G3:Cb,Ak

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 19:CLASS 21:CLASS 23:CLASS fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 13

L4 STRUCTURE UPLOADED

10/576,703 REACTION SEARCH

=> d

L4 HAS NO ANSWERS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 14 full

FULL SEARCH INITIATED 13:57:03 FILE 'CASREACT'

SCREENING COMPLETE - 2423 REACTIONS TO VERIFY FROM 251 DOCUMENTS

3 DOCS

100.0% DONE 2423 VERIFIED 5 HIT RXNS SEARCH TIME: 00.00.03

3 SEA SSS FUL L4 (5 REACTIONS)

EAST Search History

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L3	77	L2 and diketopyrrolopyrrole	US-PGPUB; USPAT; EPO, JPO, DERWENT	OR	OFF	2007/07/17 09:57